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Evaporation from sand

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Summary

A simple model for the evaporation of chemical agents from sand has been constructed, based on wind-tunnel experiments with diethylmalonate. The model is meant to be incorporated in the CHEMATT model for risk assessment.

Samenvatting

Een eenvoudig model is gemaakt voor de verdamping van strijdgassen van zand, gebaseerd op windtunnelproeven met diethylmalonate. Het model zal ingevoerd worden in het CHEMATT model voor risico analyse.

CONTENTS

1 INTRODUCTION

Equations to describe the evaporation from a (large) free liquid surface were published (ref. 3) some time ago. These are relatively simple if only the rate of evaporation is considered. To model the behaviour of drops on an absorbing surface proves to be more complex. A complete analytical solution for drops does not seem to be available. Measurements of evaporating drops also seem to be scarce. (ref. 1, 2, 3).

Recently data became available concerning the evaporation of diethylmalonate from sand. These data offer an opportunity to construct and validate a relatively simple numerical model. At our laboratory, a suite of programs is available (normally indicated as the CHEMATT model) of which one part can compute the evaporation from drops deposited on grass. This part is based on Monaghan's work. When the evaporation from sand was computed with this program, without alteration, evaporation was much too fast. This is not surprising, since Monaghan's model takes into account that the wind can blow through the space between the grass blades.

In order to simulate the evaporation from sand it is therefore necessary to model the behaviour of a drop especially for sand. In Monaghan's original report, the computation of the evaporation and subsequent dispersion was done with a set of differential equations. Although this has theoretical advantages, it seemed more practical in the CHEMATT model to treat the evaporation of the drops as a separate step. The computed rate of evaporation as a function of time is then used as input for the computation of the subsequent dispersion.

2 OBJECTIVE

The objective of this study was to construct a relatively simple model to simulate the evaporation of chemical warfare agents from sand. The method used can be applied to other data sets, if they are organized in the same way.

3 DATA DESCRIPTION

The measurements were carried out according to a fractional factorial design, which means that an attempt was made to establish the influence of some parameters on the rate of evaporation with the minimum number of tests. The investigated parameters were: windspeed, ambient temperature, drop size, viscosity, wetness of the sand, diameter of sand, relative humidity. The disadvantage of the fractional factorial design is that it assumes that the influences of the various parameters are independent of each other. In practice, the values of the parameters were:

windspeed	: 1.5 and 5.3 m/s (3 and 12 MPH)
drop diameter	: 2 and 5 mm
temperature	: 16 and 38° C (60 and 100° F)
viscosity	: 100 and 1000 centipoise
sand	: type A, B, C, D
wetness	: wet and dry
rel.humidity	: low and high (circa 25% and 60%)

Of the last two parameters, not all combinations were used

(A : ~0.4 mm diameter

B : 1.0 mm

C : 2.6 mm

D : unsieved sand 0.4 - 2.6 mm diameter

D is treated the same as C in the model)

There are 32 tests in total (see ref. 4.)

4 THE MODEL

After testing an initial and fairly arbitrary combination of Monaghan and Sutton it was attempted to use only Sutton's formula and some influence of the molecular diffusion coefficient. First an attempt was made to combine Sutton with an extra layer through which the molecules have to travel purely by Brownian motion. The transport velocity through such a layer becomes D/L (D is diffusion coefficient taken as 7.4E-5 m^2/s and L is thickness of the layer). Comparison with the experiments shows that a good fit is obtained if the layer is chosen as 2 times the maximum grain size (see Table 1). This picture presupposes that the liquid gets back to the surface by the capillary forces leaving only a thin layer to be crossed by the vapour.
In this model the liquid is assumed to have the form of a spherical segment that keeps its form when it gets smaller.
Also the experimental spread factor of 2.7 is used throughout.
Since neither of the previous simulations describe the very slow evaporation that often seems to occur after the half-way point, a third approach was tried. In this case it is assumed that the drop does not stay attached to the surface. Now a growing layer forms between the top of the sand and the top of the drop. For the moment, a transport velocity is assumed equal to D/L, but multiplied by the porosity to account for the fact that it is not an open layer. It still has to be looked into whether this transport is close enough to reality. The results of these computations are remarkably close to those of Table 1. Table 2 gives the three sets of answers in one table.

Table 1 Measured and computed half-life in seconds

Nr	Sutton + Layer Computed	Experiment	Sand type
S1	20000	30000	A wet
S2	48000	66000	C dry
S3	65000	>100000	B wet
S4	120000	>120000	D dry
S5	40000	24000	D wet
S6	20000	19000	B dry
S7	100000	85000	C wet
S8	30000	54000	A dry
S9	50000	45000	D wet
S10	30000	45000	B dry
S11	130000	>100000	C wet
S12	55000	90000	A dry
S13	12000	10800	A wet
S14	40000	43000	C dry
S15	46000	40000	B wet
S16	100000	>100000	D dry
S1D	8000	12000	A wet
S2D	18000	>24000	C dry
S3D	27000	30000	B wet
S4D	45000	36000	D dry
S5D	14000	5400	D wet
S6D	7000	4200	B dry
S7D	35000	17000	C wet
S8D	11000	12000	A dry
S9D	17000	16000	D wet
S10D	10000	10000	B dry
S11D	43000	23000	C wet
S12D	20000	24000	A dry
S13D	4300	4500	A wet
S14D	14000	6000	C dry
S15D	16000	9000	B wet
S16D	35000	15000	D dry

Table 2 Comparison of computed and experimental values

Sutton+Monaghan = Modified Monaghan model

Sutton+layer = Sutton + molecular diffusion

Sutton+ 2 layers = Sutton + molecular diffusion and drop detached from surface

Experiment	Sutton+Monaghan Computed	Sutton+Layer Computed	Sutton + 2 Layers Computed
30000	28000	20000	23000
66000	28000	43000	50000
>100000	60000	65000	77000
>120000	70000	120000	125000
24000	10000	40000	40000
19000	10000	20000	20000
85000	25000	100000	110000
54000	25000	30000	40000
45000	40000	50000	50000
45000	30000	30000	30000
>100000	90000	130000	140000
90000	85000	55000	60000
10800	10000	12000	14000
43000	10000	40000	40000
40000	30000	46000	58000
>100000	30000	100000	110000
12000	11000	8000	8000
>24000	11000	18000	18000
30000	32000	27000	30000
36000	32000	45000	50000
5400	4000	14000	15000
4200	4000	7000	7000
17000	10000	35000	38000
12000	10000	11000	14000
16000	10000	17000	18000
10000	10000	10000	11000
23000	25000	43000	47000
24000	25000	20000	22000
4500	4000	4300	4800
6000	4000	14000	15000
9000	10000	16000	21000
15000	10000	35000	38000

It was found that this third approach cannot explain the very slow evaporation during the second half of the process either.

In order to explain the second half, one has to assume that another process is at work. The most obvious candidate for this is the diffusion or absorption of agent into the sand. Since we cannot distinguish between different ways in which the agent could move through the sand, the process is treated here as a transport of vapour into the sand with a transport velocity Vsink. This would lead to the conclusion that one really needs something like Monaghan's absorption velocity. This would then have to be considered as a process going on at the same time and in competition with the evaporation into the atmosphere.

Another assumption could be that always a fixed percentage is absorbed in the sand. This would probably fit well to at least half of the present data, but the approach with a Vsink is more flexible. In Monaghan's work however, there are indications that a Vsink would be different for different agents, which would require extra tests for other agents.

After these initial runs, the effort was concentrated on the following combination :

- Use Sutton's equation to account for the atmospheric transfer rate;
- Introduce a layer through which the vapour has to move by molecular diffusion and make this layer dependent on the grain size of the sand;
- Introduce a Vsink to account for absorption of agent into the sand;
- Retain the feature of the shrinking drop of constant shape.

In the program, an effective sand diameter is introduced:

$$\text{Diazeff} = \text{intercept} + \text{Facdiam}*\text{Diam} + \text{Facdry}*\text{Drypoint}$$

Drypoint is a parameter that is equal to 1 for tests with dry sand and equal to 0 for tests with wet sand. The three parameters, intercept, Facdiam, and Facdry are later determined by fitting the model to the test data.

In the present program, the spread factor of 2.7 according to Cooper's report was used. It was further assumed that the drop , after being sucked up by the sand, has the form of half a sphere, but a spherical segment of smaller height could also be used. This corresponds to assuming that the volume of the pores is the fraction 'poriefac' with

$$\text{poriefac} = 2 / SF^3$$

The transfer rate through the thin top layer of the sand, through which the vapour has to pass by molecular diffusion, is taken as:

Vsand = Difco * poriefac / Diazeff

Difco = 7.4E-5 m^2/s (molecular diffusion coefficient)

(N.B. As mentioned above the atmospheric transfer rate is
Vsutton = 0.0027 * $UW^{0.78}$ * $X0^{(-0.11)}$)

The combined transfer rate :

Veff = Vsutton*Vsand / (Vsutton+Vsand)

The loss of material from the drop into the atmosphere is calculated in time steps dt :

loss = Veff*Satcon*PI*$Diaz^2$ * dt /4

The loss into the sand is calculated as

loss = Satcon*Vsink*PI*$Diaz^2$ /2 * dt

(the surface of a sphere is PI*D^2)

In the simulation, the loss of mass and the resulting smaller diameter are alternately calculated until the drop disappears. Also the amount of material transferred to the atmosphere is subtracted from the total amount giving the fraction remaining at every time step.

5 RESULT OF THE FIT

The resulting model data are compared with the experimental data for a limited number of points per test (6 - 7 points per test). The differences are squared and accumulated for the points and also for all 32 tests.
In order to find the best values for the parameters, a searching program was employed that can repeat the whole computation for different values of the critical parameters. Using this technique, a value for Vsink was found of 0.0003 m/s (relative to vapour), and for the layer mentioned above, the result was :

$$\text{diazeff} = 0.54 + 0.41 * \text{Diaz} + 0.58 * \text{Drypoint}$$

where Drypoint = 0 for wet sand and Drypoint = 1 for dry sand.

For the time being this seems to be the best obtainable fit. It has also been tested whether there was any influence of the relative humidity, but no improvement in the model fit was found by taking this into account. Figures have been made of the 32 measured evaporation curves and their model fit. Although for most tests, experiments and model fit quite well, there are a few notable exceptions that cannot be explained at the moment.
The fit gives about 7% as the overall accuracy. Since all curves start at a value of 1, this value should be doubled to 14% to give a realistic impression of the accuracy.
A computer program has been written that implements the model and fit as described in this report.

6 RETENTION OF AGENT IN SAND

The amount of agent that seems to remain in the sand when the rate of evaporation has dropped to zero is an interesting figure in its own right. Although this amount often seems significantly above zero, there are indications that this may be an artifact of the tests: in many cases the tests were stopped long before the rate of evaporation was zero.
If, however, this amount is roughly estimated from the graphs then there seems to be some retention in the sand at a time when an observer may think that most agent has disappeared.
This can be studied making use of the fractional factorial design. Statistical analysis yields:

diameter	: no influence	
viscosity	: no influence	
temperature	: influence	16 C --> 36% retention (average)
		38 C --> 20% retention
sand diameter	: influence	0.4 mm --> 22% retention
		1.0 mm --> 23%
		2.6 mm --> 34%
wetness	: no influence	
windspeed	: no significant influence	

7 CONCLUSION

By combining the rate of evaporation from a free liquid surface (Sutton) with an extra layer through which the vapour must pass by molecular diffusion, and with a Vsink to account for the absorption of agent into the sand, an accurate description of the present evaporation trials can be given. There are aspects to this problem however that may require more tests, notably the expected dependence of Vsink on the agent. It is expected that other substrates will lead mainly to different absorption rates, but that the initial rate of evaporation may not differ significantly. Since the initial rate of evaporation determines the immediate hazard, the present sand data are probably also representative for the hazard on many other substrates.

8 AUTHENTICATION

C.J.P. van Buytenen
(Author)

9 REFERENCES

1 Monaghan, J. and McPherson, W.R.
"A mathematical model for predicting vapour dosages on and downwind of contaminated areas of grassland"
Suffield Technical Paper No. 386, Sept. 1976

2 Chinn, K.S.K.
"A simple method for predicting chemical agent evaporation"
U.S. Army Dugway Proving Ground, report DPG-TR-401, Sept.1981

3 Sutton, O.G.
"Micrometeorology"
McGraw Hill Publ. Co. Ltd. London, 1953

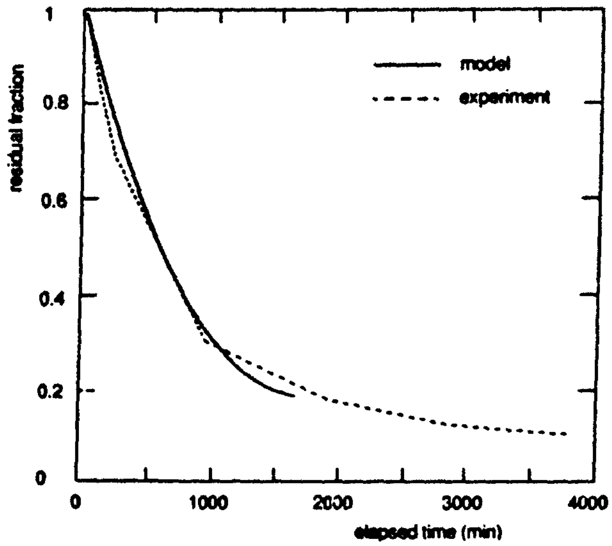
4 Cooper, W.A.
"Evaporation of a thickened agent simulant from wet and dry sand"
Report CRDEC-TR-112, Feb. 1990
CRDEC, Aberdeen Proving Ground, Maryland 21010-5423

5 Medema, J. and Buijtenen, C.J.P. van
"Calculation of the vapour dosage downwind from a contaminated source"
Report PML-TNO 1986-37

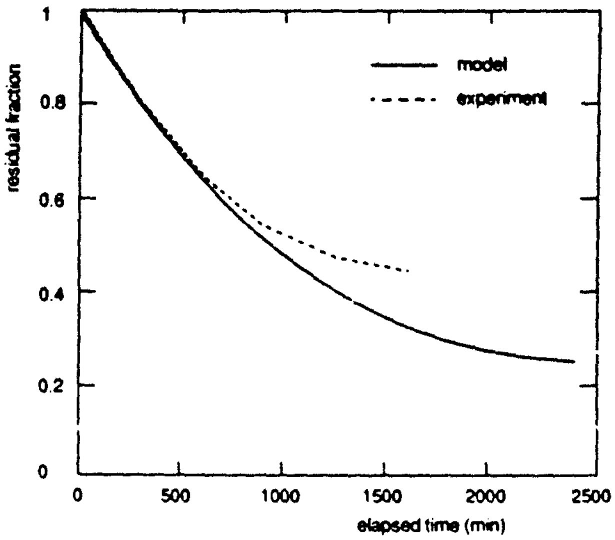
6 "Methods for the computation of the physical effects of the accidental release of dangerous chemicals "
Report prepared by The Netherlands Research Organization
TNO for the Ministry of Social Affairs, Directorate General of Labour, Voorburg, 1988

ANNEX 1 GRAPHS FOR SAND DATA

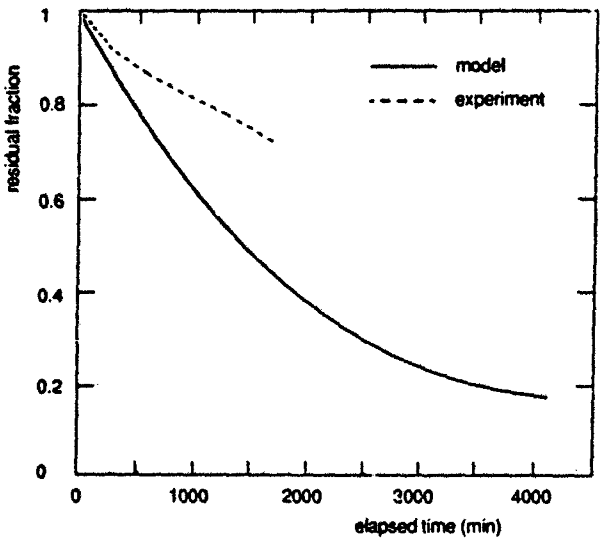
(All 32 graphs)



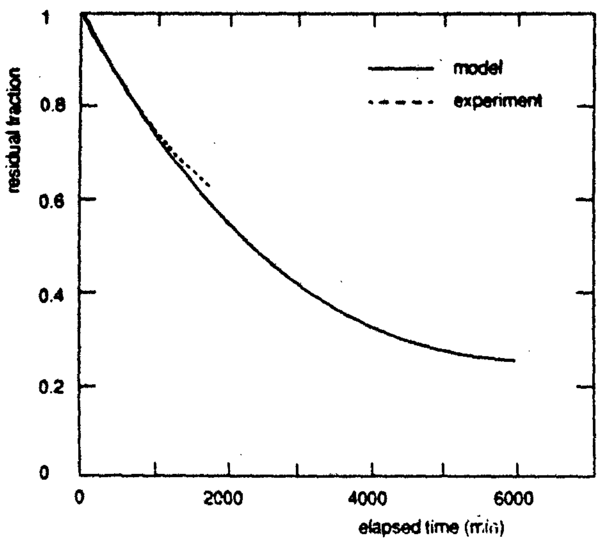
Test : S1C Windspeed = 1.5 m/s Error = 5.55
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m^3
Sand : A-WET Visc = 60 cp Temp = 60 F



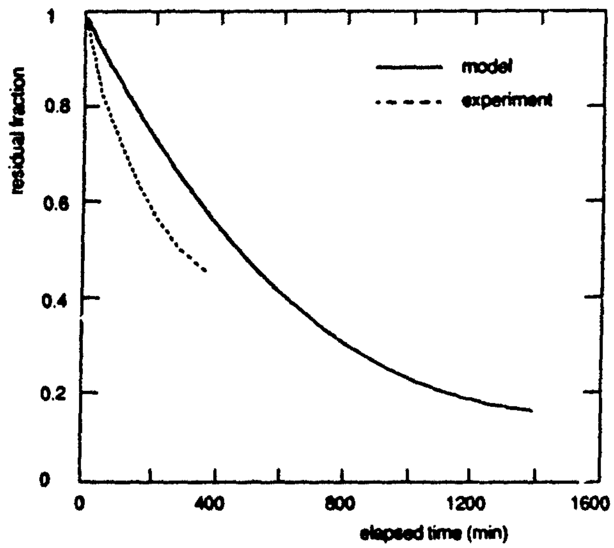
Test : S2C Windspeed = 1.5 m/s Error = 5.85
Drop Diam. = 2 mm Sat Vap = 1.5 g/m^3
Sand : C-DRY Visc = 100 cp Temp = 60 F



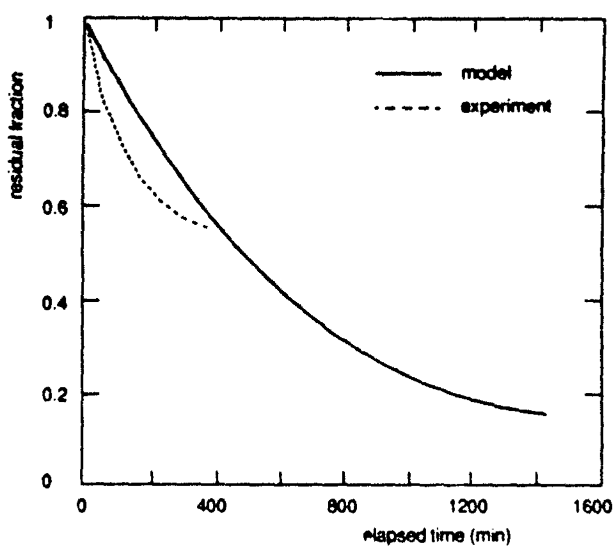
Test : S3C Windspeed = 1.7 m/s Error = 19.0
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : B-WET Visc = 100 cp Temp = 60 F



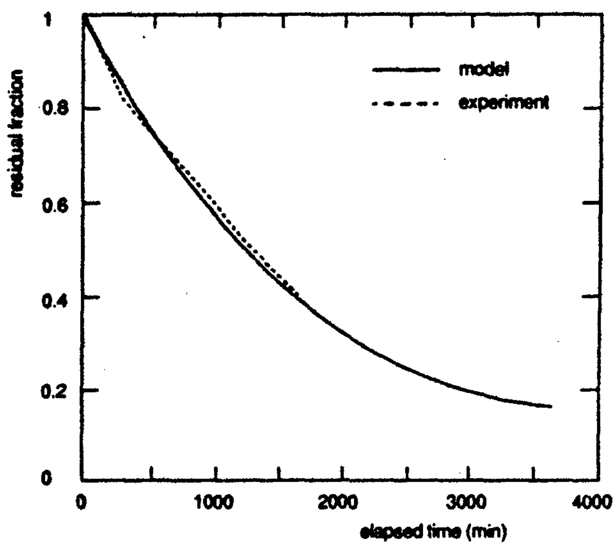
Test : S4C Windspeed = 1.6 m/s Error = 1.76
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : D-DRY Visc = 100 cp Temp = 60 F



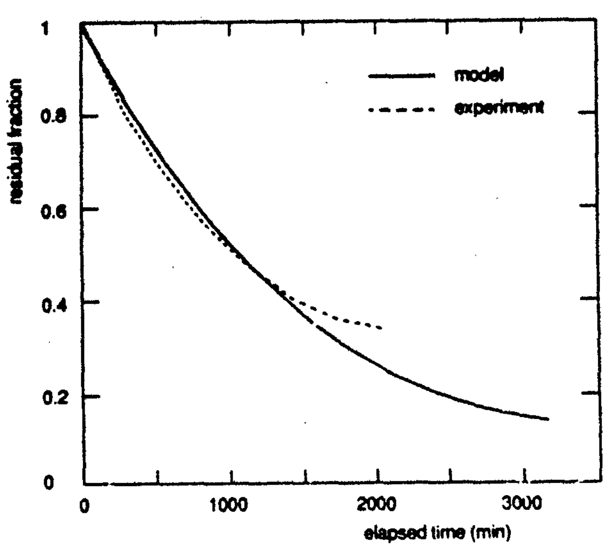
Test : S6C Windspeed = 5.3 m/s Error = 13.6
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m^3
Sand : B-DRY Visc = 100 cp Temp = 60 F



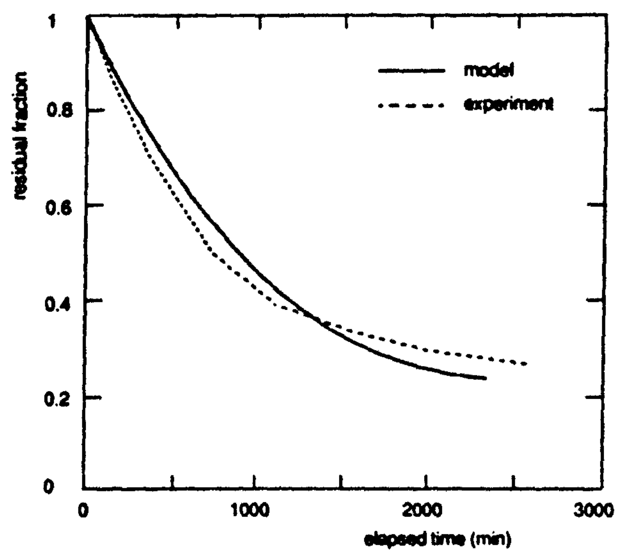
Test : S5C Windspeed = 5.3 m/s Error = 9.86
Drop Diam. = 2 mm Sat Vap = 1.5 g/m^3
Sand : D-WET Visc = 100 cp Temp = 60 F



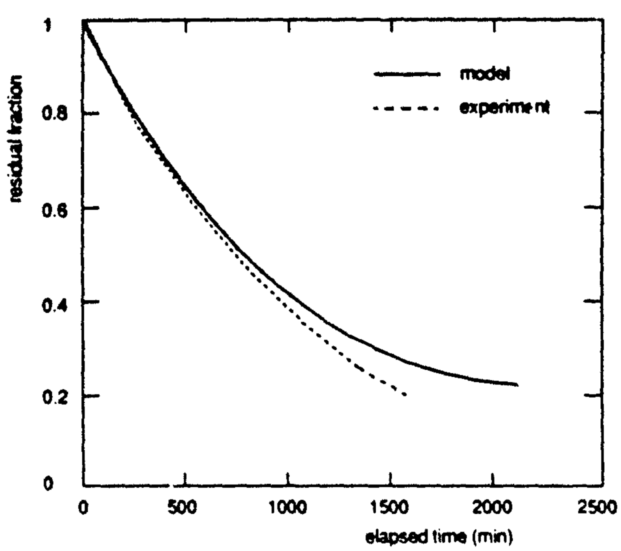
Test : S7C Windspeed = 5.3 m/s Error = 1.89
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : C-WET Visc = 100 cp Temp = 60 F



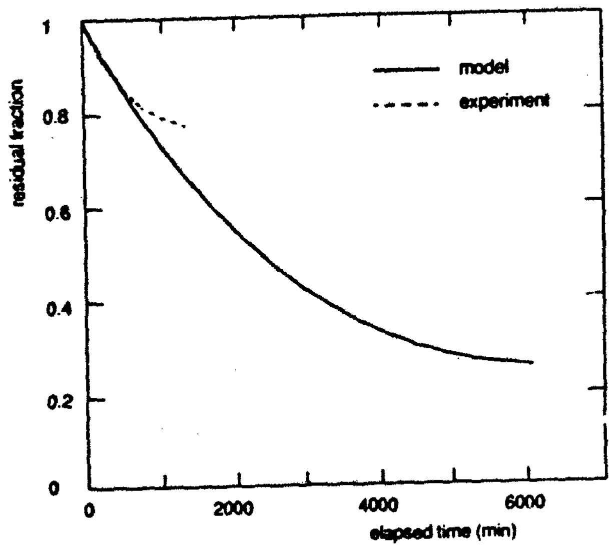
Test : S8C Windspeed = 5.3 m/s Error = 4.07
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : A-DRY Visc = 100 cp Temp = 60 F



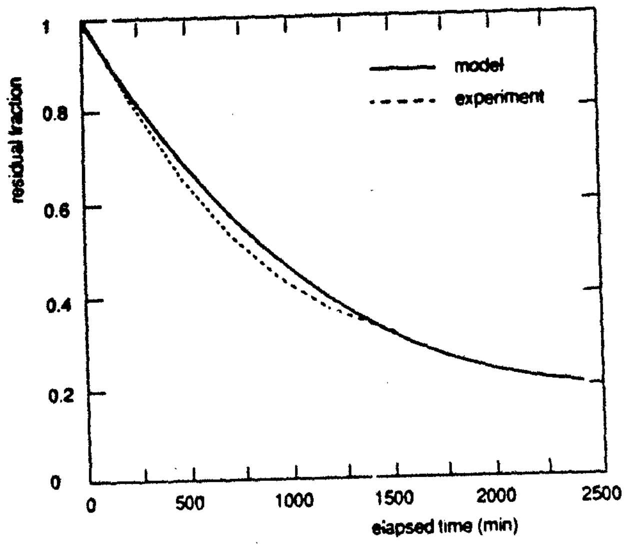
Test : S9C Windspeed = 1.2 m/s Error = 3.87
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m^3
Sand : D-WET Visc = 1000 cp Temp = 60 F



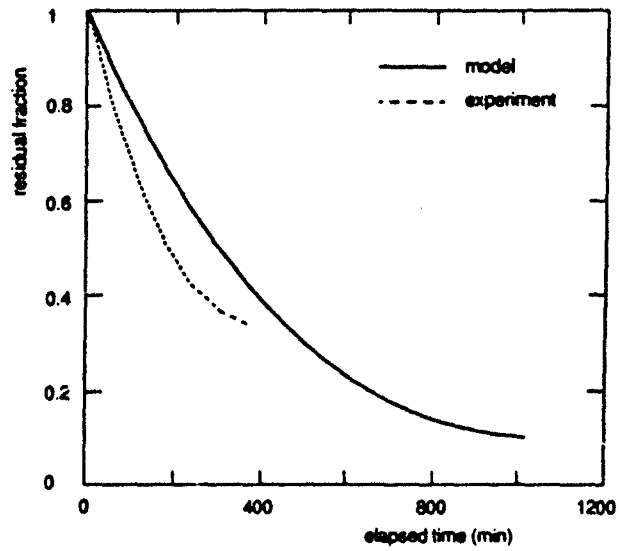
Test : S10C Windspeed = 1.5 m/s Error = 4.28
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m^3
Sand : B-DRY Visc = 1000 cp Temp = 60 F



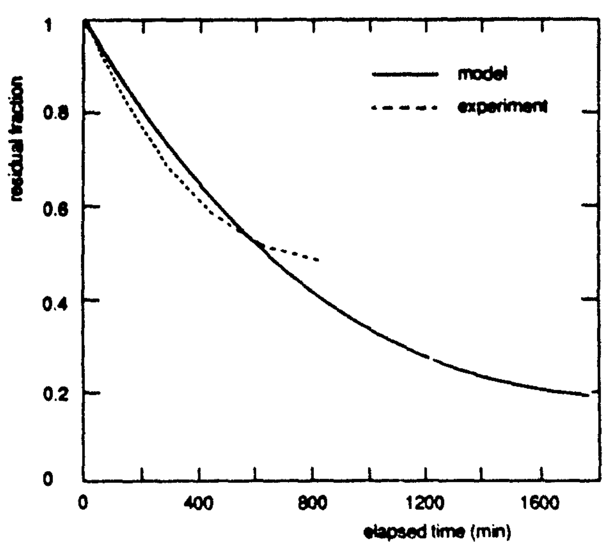
Test : S11C Windspeed = 1.1 m/s Error = 5.32
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : C-WET Visc = 1000 cp Temp = 60 F



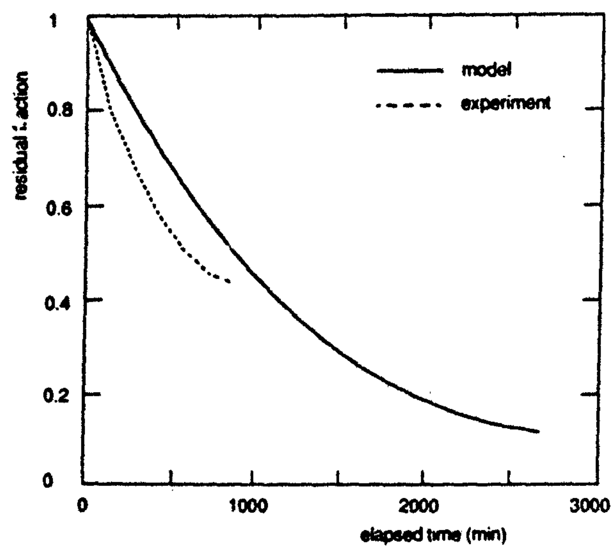
Test : S12C Windspeed = 1.5 m/s Error = 2.99
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : A-DRY Visc = 1000 cp Temp = 60 F



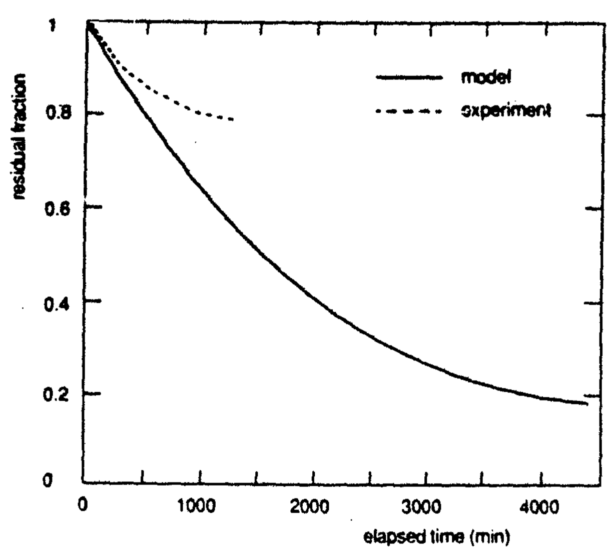
Test : S13C Windspeed = 5.3 m/s Error = 13.0
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m3
Sand : A-WET Visc = 1000 cp Temp = 60 F



Test : S14C Windspeed = 5.3 m/s Error = 4.35
Drop Diam. = 2 mm Sat.Vap = 1.5 g/m3
Sand : C-DRY Visc = 1000 cp Temp = 60 F



Test : S15C Windspeed = 5.3 m/s Error = 11.2
Drop Diam. = 5 mm Sat.Vap = 1.5 g/m^3
Sand : B-WET Visc = 1000 cp Temp = 60 F



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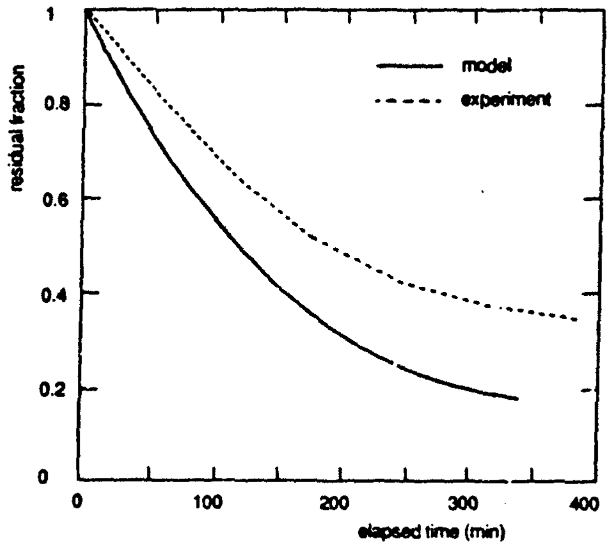
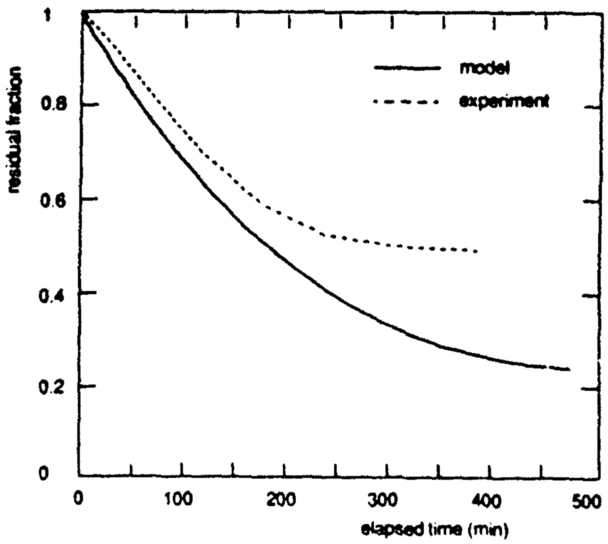
Sand : D-DRY Visc = 1000 cp Temp = 60 F



Test : S1D Windspeed = 1.4 m/s Error = 15.6
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m^3
Sand : A-WET Visc = 100 cp Temp = 100 F



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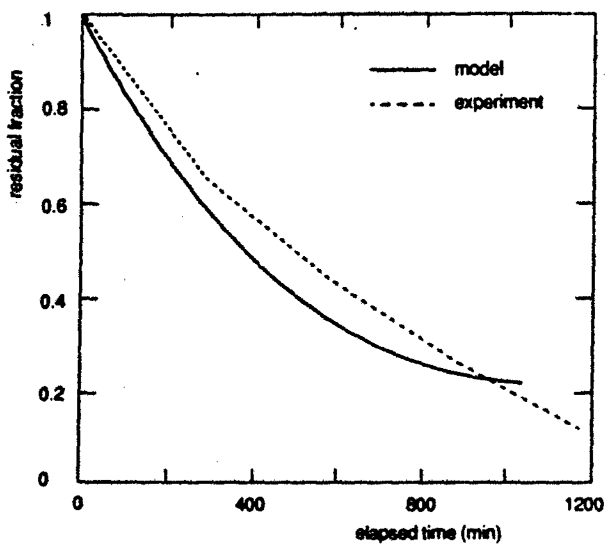
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m^3
Sand : C-DRY Visc = 100 cp Temp = 100 F



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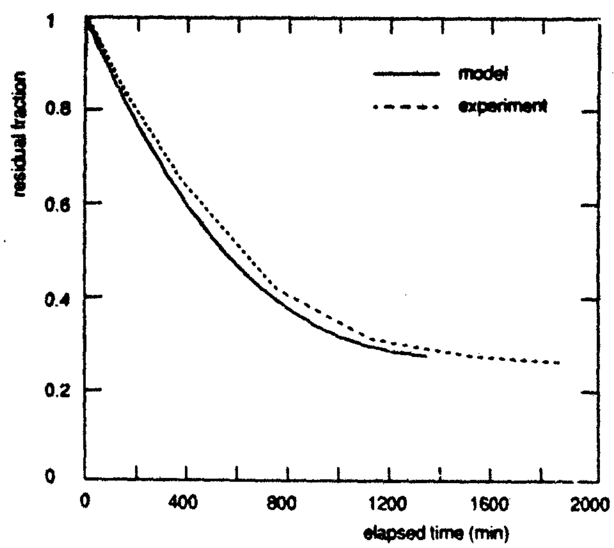
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : B-WET Visc = 100 cp Temp = 100 F



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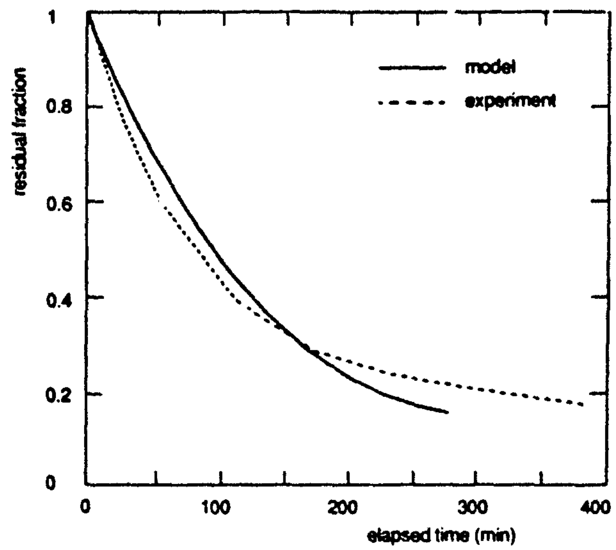
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : D-DRY Visc = 100 cp Temp = 100 F



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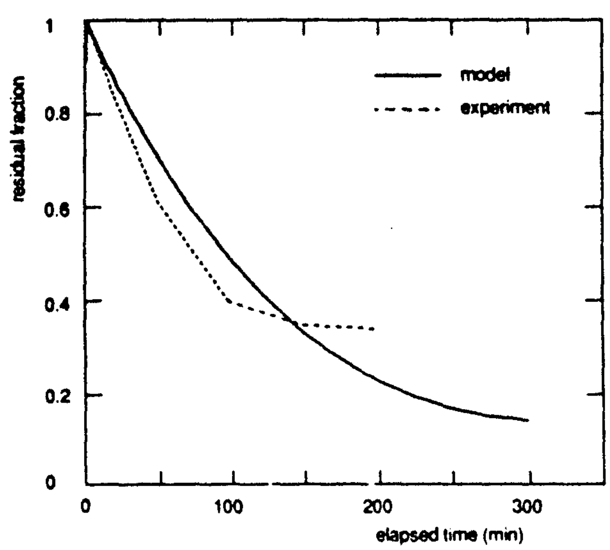

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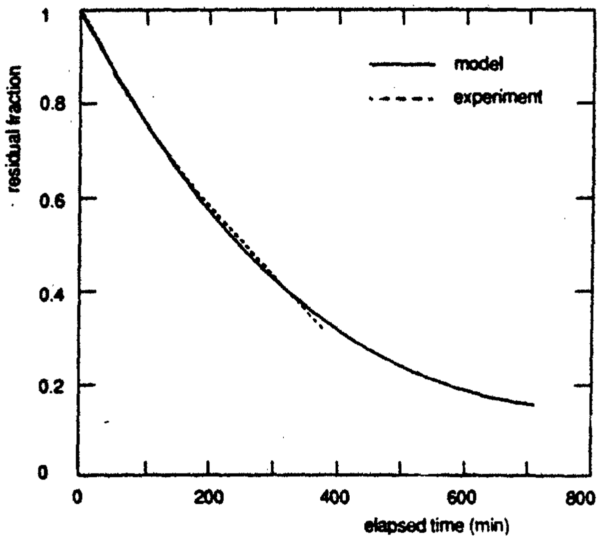
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m^3
Sand : B-DRY Visc = 100 cp Temp = 100 F



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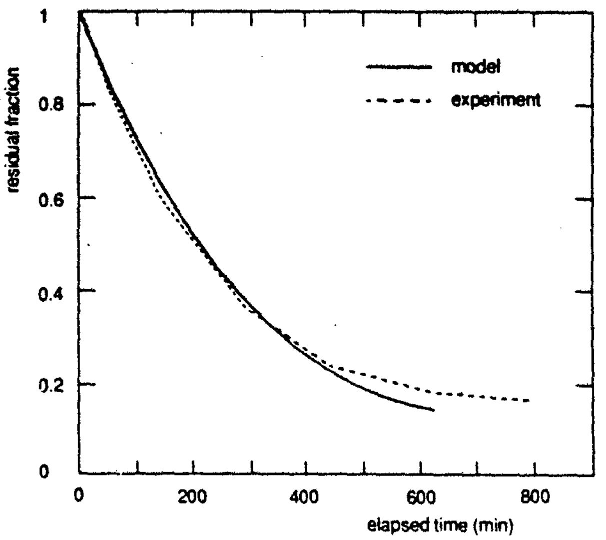
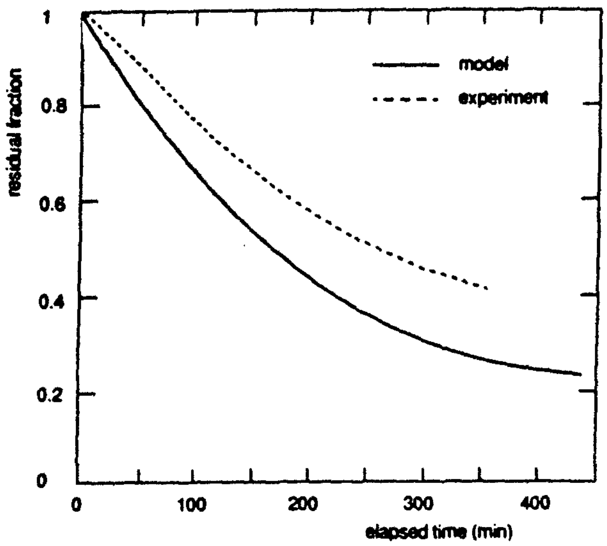
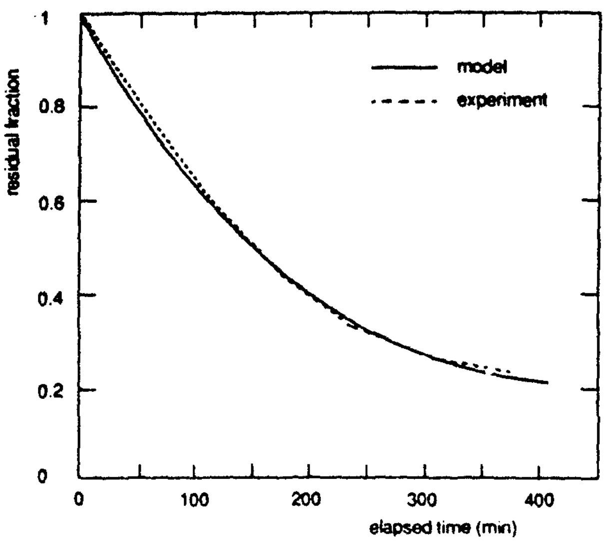
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m3
Sand : C-WET Visc = 100 cp Temp = 100 F



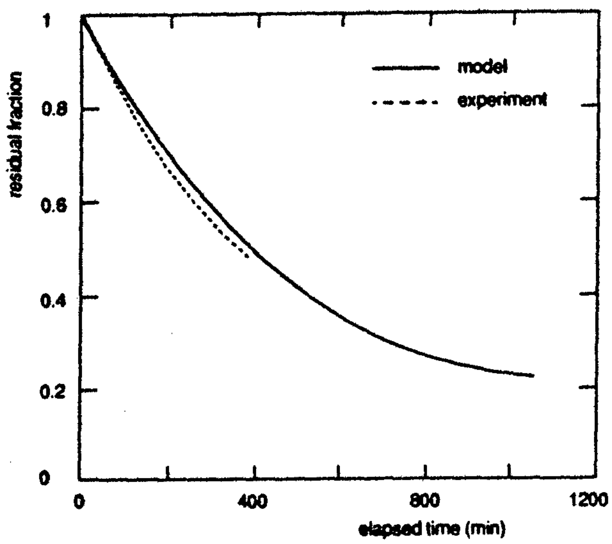
Test : S8D Windspeed = 5.3 m/s Error = 2.50
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m3
Sand :A-DRY Visc = 100 cp Temp = 100 F



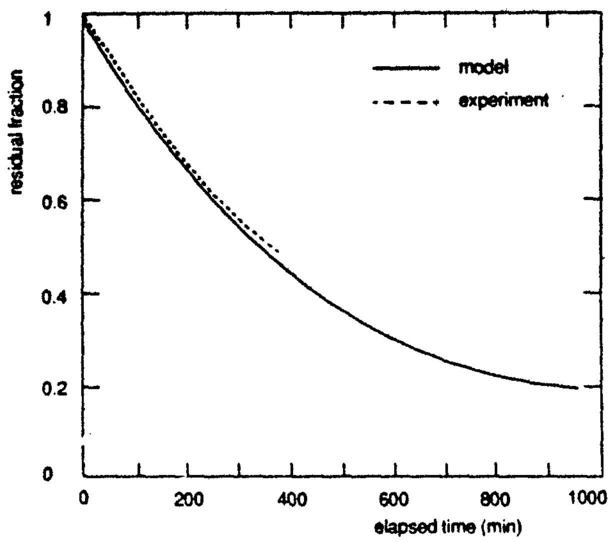
Test : S9D Windspeed = 1.4 m/s Error = 13.0
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m3
Sand : D-WET Visc = 1000 cp Temp = 100 F



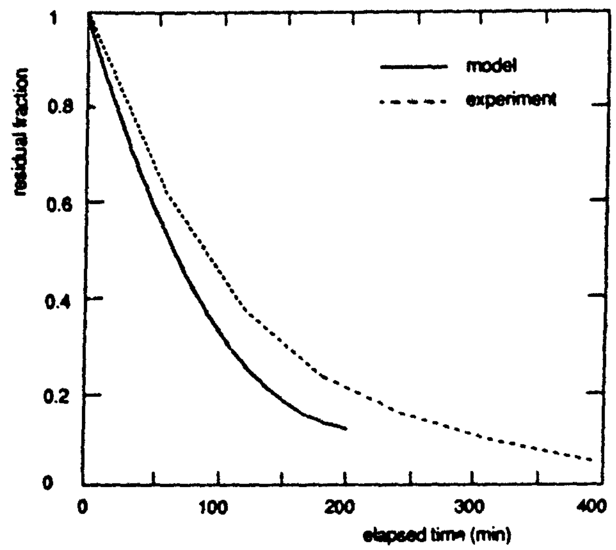
Test : S10D Windspeed = 1.5 m/s Error = 1 26
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m3
Sand : B-DRY Visc = 1000 cp Temp = 100 F



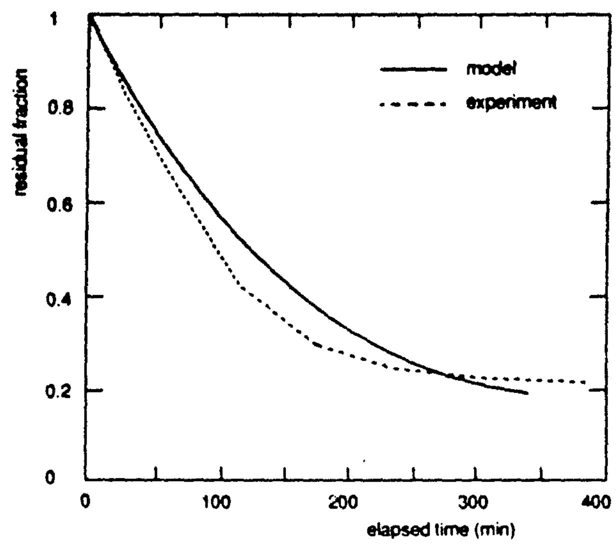
Test : S11D Windspeed = 1.5 m/s Error = 2.78
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : C-WET Visc = 1000 cp Temp = 100 F



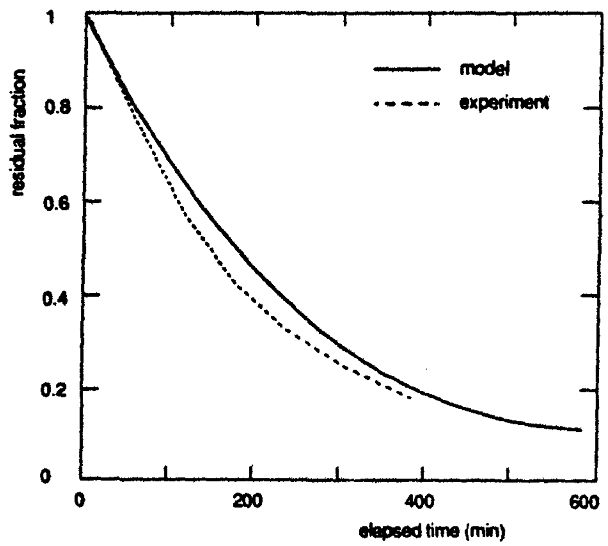
Test : S12D Windspeed = 1.5 m/s Error = 1.£2
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : A-DRY Visc = 1000 cp Temp = 100 F



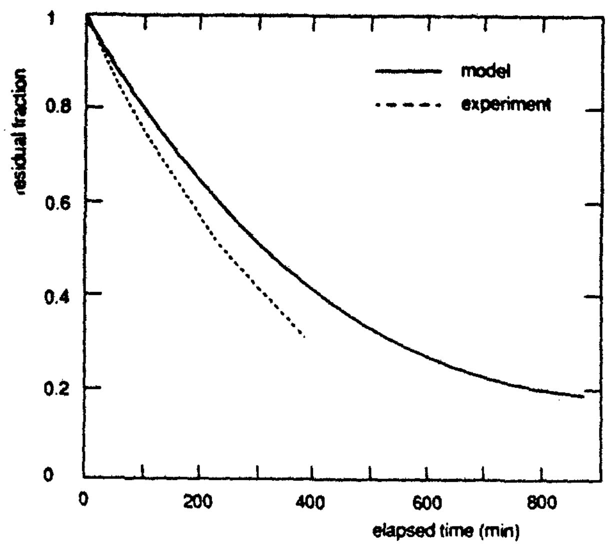
Test : S13D Windspeed = 4.9 m/s Error = 8.06
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m^3
Sand : A-WET Visc = 1000 cp Temp = 100 F



Test : S14D Windspeed = 5.3 m/s Error = 5.42
Drop Diam. = 2 mm Sat.Vap = 7.5 g/m^3
Sand : C-DRY Visc = 1000 cp Temp = 100 F



Test : S15D Windspeed = 5.2 m/s Error = 5.20
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : B-WET Visc = 1000 cp Temp = 100 F



Test : S16D Windspeed = 5.3 m/s Error = 7.93
Drop Diam. = 5 mm Sat.Vap = 7.5 g/m^3
Sand : D-DRY Visc = 1000 cp Temp = 100 F

ANNEX 2 EVAPORATION FROM CONCRETE

Data are also available on the evaporation from concrete. The experiments were done in the same way as for sand (in fact the concrete test were done earlier), i.e. as a fractional factorial design of 32 tests. There were two levels for the following variables:

- Agents : DEM and MES (Diethylmalonate and MethylSalicylate);
- Temp : 60 and 100 ° F;
- Viscosity : 100 and 1000 centipoise;
- Wind speed : 4 and 12 MPH (circa 1.7 and 5.3 m/s);
- Diameter : 2 and 5 mm drops were used.

There were four degrees of wetness of the concrete:

- type D : dry;
- type I : initially wet;
- type N : wet but no constant water table;
- type C : wet and constant water table.

There are some general trends recognizable in the influence of the parameters (see report by J. Jensen, Jaycor). In short, he found that for the initial rate of evaporation, which is probably the part that interests us most, the following influences could be computed:

Drop size : rate 2 mm / rate 5 mm = 1.57
This is less than expected. The ratio is not influenced by windspeed, agent or temperature.
Slight influence of viscosity

Agent : DEM/MES = 1.83
No influence of Drop size, viscosity
Some influence of windspeed, temperature

Temperature : rate 100°F/rate 60°F = 2.56
This is lower than expected, which indicates cooling of the concrete especially when wet.
No influence : windspeed, drop size, viscosity
Influence : Agent, wetness of concrete

Wind speed : rate 12 mph/rate 4 mph = 2.16
About as expected (: $U^{0.7}$)
No influence: Drop size, temperature, agent, viscosity
Influence : wetness ??

Viscosity : 100cp/1000cp = 1.71
No influence of windspeed, agent, Drop size, temperature
Influence : ??

The relative humidity seems to have no clear influence on the evaporation.

Most of these influences are handled in a straightforward way by a relatively simple model, except viscosity, which could work through the spread factor. There was, however, no experimental evidence of this.

Retention in concrete

The same methods as for sand were applied to the data for concrete. According to the stepwise multiple regression, none of the parameters gave a significant regression coefficient.

The analysis of variance indicates that there is a slight influence of drop diameter and windspeed, but the influence has a lower significance than is normally used.

Drop diameter influence:

2 mm --> 24% retention (st. dev. 3%)
5 mm --> 16.5% retention (st. dev. 3%)

Windspeed influence :

1.8 m/s --> 16.7% retention (st. dev. 2.6%)

5.3 m/s --> 24.3% retention (st. dev. 3.3%)

Viscosity, temperature, wetness, agent-type and relative humidity seem to have no significant influence at all

ANNEX 3 MODEL FOR EVAPORATION FROM CONCRETE

After some trial and error the following model description was used: the drops start as a cylinder with a diameter of 5 times (= spread factor) the original diameter. The diameter stays constant for a time deduced from Monaghan's formula :

Tconstant = CD/(5.5*Cs*(V1+V0))

where

CD = contamination density = liquid loading;

Cs = saturated vapour concentration;

V1 = transfer rate for vapour from the top;

V0 = transfer rate into the bottom (Vsink).

After the constant period the drop shrinks, but keeps the same shape. As already suggested by the above formula, part of the vapour is transferred to the atmosphere (Vsutton), and part is transferred to the concrete (Vsink).

(Vsutton = $0.0027 \cdot U^{0.78}$ (see ref. 6.))

After the whole mass of the drop has disappeared, vapour very slowly evaporates from the concrete. During the last phase, the vapour has to travel through a layer of concrete that at first is zero, but slowly grows as time goes by. This further slows down the last phase. It is assumed that this process starts right from the beginning. At first it has little influence because the initial rate of evaporation is much faster, but it helps to build up a value for the layer of concrete through which the vapour has to go in the last stage.

By fitting the model to the data, using the method of Powell, the following parameters were determined:

CORRFACU = 0.67 : correction on Sutton's constant 0.0027;

CORRFACS = 0.706 : correction for cooling of the concrete;

FACV = 2.25E-5 : correction for the porosity of the concrete
transfer rate = FACV*DIFCO (DIFCO=0.000074 m2/sec);

FACT = 1.5 :correction to Tconstant acc. to Monaghan;

Vsink = 0.00155 m/s.

In Sutton's equation, a power of 0.7 gives a slightly better fit than 0.78. The reason for this is not quite clear, but Sutton's value was determined for a different kind of surface (grass), which can easily influence the transfer rate.

When the model is compared with the data, it is clear that the fit for concrete is much worse than for sand.

For the fit presented here, especially tests 3, 5, 11, 15, 19, 21, 26, and 31 deviate strongly from the model. It seems, however, impossible to relate the deviation to the different parameters because the deviations are not supported by other tests with the same parameters. From the "bad" cases, 5 are of type I , 2 are D and 1 is N. This suggests that perhaps the degree of wetness is the parameter that causes the deviations, because "Initially wet" is probably not a very well-defined condition. Two cases of D (for dry) could mean that for dry concrete differences in porosity may show up more than for wet concrete. It seems clear from the comparison of the model with the data, that there are inconsistencies in the data.

The accuracy indicated by the fit is 9.9 % without the 8 bad tests and 13.6 % including those 8. In order to obtain a realistic impression of the accuracy one should multiply this figure by 2 since all the curves start at the point 0,1 and therefore the error at the start is always zero.

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A simple model for the evaporation of chemical agents from sand has been constructed, based on wind-tunnel experiments with diethylmalonate. The model is meant to be incorporated in the CHEMATT model for risk assessment.

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